Dibromomethane

74-95-3 | DTXSID4021557

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -46.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.05e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

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Dibromomethane Measured: -52.5 Predicted: -46.0

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Ethylidene bromide Measured: -63.0 Predicted: -39.7

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1,2-Dibromoethane Measured: 9.90 Predicted: -25.6

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1,3-Dichloropropene Measured: -50.0 Predicted: -46.1

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(Z)-Dichloropropene Measured: -50.0 Predicted: -46.1

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(Z)-1,2-Dichloroethylene Measured: -64.9 Predicted: -69.7

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(E)-1,2-Dichloroethylene

Measured: -64.9 Predicted: -69.7